Max-Planck-Institut
für Mathematik
in den Naturwissenschaften
Leipzig

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by

Carl Friedrich Kreiner, Johannes Zimmer, and Isaac Chenchiah

Preprint no.: 94 2003

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C.-F. Kreiner*, J. Zimmer*, I.V. Chenchiah†

* Max Planck Institute for Mathematics in the Sciences,
Inselstr. 22, 04103 Leipzig, Germany
† Division of Engineering and Applied Science,
California Institute of Technology, Pasadena CA 91125, USA

Abstract

The problem of detecting so-called T_k-configurations is addressed here. These configurations are the most prominent examples of sets with nontrivial rank-one convex hulls. Rank-one convex hulls play an important rôle in the calculus of variations and the modelling of effective properties of materials.

An efficient algorithm, based on algebraic methods, is presented. Unlike previous work on the computation of rank-one convex hulls, it is not based on discretization and gives exact results. This algorithm enables, for the first time, large numbers of tests for these configurations. Stochastic experiments in several space dimensions are reported here.

1 Introduction

This paper addresses the efficient algebraic detection of so-called T_k-configurations (see Definition 2.1 below), which are the most prominent examples of non-trivial rank-one convex hulls. Rank-one convex hulls of sets and rank-one convex envelopes of functions are important notions in the calculus of variations [10]. Further, the rank-one convex envelope of a nonconvex microscopic energy function of a material serves as a model for its macroscopic energy, which explains the relevance of rank-one convexity to engineering and the importance of a reliable method for the computation of these hulls and envelopes.

Previous algorithms for the computation of the rank-one convex hull of a set $\mathcal{M} \subset \mathbb{R}^{m\times n}$ have been based on a discretization of the space and the rank-one convexification of the distance function $d(x) := \min_{y\in\mathcal{M}} \|x - y\|$ along finitely many rank-one directions [1, 2, 3]. The complexity of these algorithms is high. The results depend very sensitively on the chosen discretization and especially on the choice of rank-one directions. Moreover, satisfactory results typically require a high degree of precision. It is easy to see that such a discretization-based algorithm will fail completely if essential rank-one lines are missed. An example of a numerical instability is given in [9].

In this paper, we study a simpler, but closely related and important question rigorously. Specifically, we answer a question posed in [6, Section 8] by presenting an efficient algorithm for the detection of T_k-configurations as an important example of nontrivial rank-one convex hulls. The guiding idea is to exploit the algebraic structure of rank-one convexity.

2 T_k-configurations and their algorithmic detection

We start with the definition of T_k-configurations.

Definition 2.1 *A finite set* $\mathcal{M} = \{M^{(1)}, M^{(2)}, \dots M^{(k)}\} \subset \mathbb{R}^{m\times n}$ *of* $k \geq 4$ *matrices is called a* T_k-configuration *if there exist a permutation* σ *of* $\{1, \dots, k\}$, *rank-one matrices* $C^{(1)}, C^{(2)}, \dots, C^{(k)} \in \mathbb{R}^{m\times n}$, *positive scalars* $\kappa_1, \kappa_2, \dots, \kappa_k$, *and matrices* $X^{(1)}, X^{(2)}, \dots, X^{(k)} \in \mathbb{R}^{m\times n}$ *such that the relations*

$$X^{(j+1)} - X^{(j)} = C^{(j)}, \qquad M^{(\sigma(j))} - X^{(j+1)} = \kappa_j C^{(j)} \tag{1}$$

hold, where the index j is counted modulo k (see Fig. 1). □

This differs only slightly from the definition in [6, Definition 7] where $\mathcal{M}$ is considered as a tupel rather than as a set (i.e., $\sigma = \text{id}$).

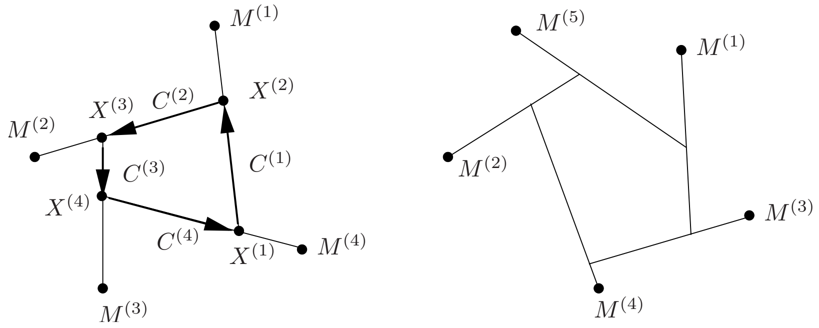

Figure 1: A T_4-configuration and a T_5-configuration, both projected to $\mathbb{R}^2$.

A *degenerated T_k-configuration* arises as limit of T_k-configurations where the inner polygon formed by the $X^{(j)}$ reduces to a single point. More precisely, there exists an $X \in \mathcal{M}^{co}$ (the usual convex hull of $\mathcal{M}$) with $\text{rank}(X - M^{(j)}) = 1$ for all $M^{(j)} \in \mathcal{M}$.

We state some connections between T_k-configurations and rank-one convex hulls. For a set $\mathcal{M} \subset \mathbb{R}^{m\times n}$, the rank-one convex hull will be denoted by $\mathcal{M}^{rc}$ (see, e.g., [10] for the precise definition).

It is easy to verify that the rank-one convex hull of a T_k-configuration $\mathcal{M}$ (indexed such that $\sigma = \text{id}$) contains at least $\bigcup_{j=1}^{k}[M^{(j)}, X^{(j)}]$, where $[A, B]$ is the line segment between A and B. For a degenerated T_k-configuration, one has $\bigcup_{j=1}^{k}[M^{(j)}, X]$, see [7, Corollary 4.19]. Note that, unlike in the classical example given by Tartar [14], $\mathcal{M}$ need not lie in a plane, even for $k = 4$.

The question asked in [6, Section 8] and addressed here can be phrased as follows. *Let $k \geq 4$ matrices $M^{(1)}, \ldots, M^{(k)} \in \mathbb{R}^{m\times n}$ without rank-one connections (i.e., $\text{rank}(M^{(i)} - M^{(j)}) \geq 2$ for $i \neq j$) be given. Do they form a T_k-configuration?*

We will study only the interesting case $k \geq 4$, since T_3-configurations lie necessarily in a plane consisting of rank-one lines. The stochastic experiments in Section 3 will concentrate on T_4-configurations. In the special case of $\mathbb{R}^{2\times 2}$, the T_4-configurations are in some sense the universal example for finite sets with nontrivial rank-one convex hull. This is due to the following theorem [13, Theorem 2].

Theorem 2.2 (Székelyhidi, '03) *Let $\mathcal{M} \subset \mathbb{R}^{2\times 2}$ be a compact set without rank-one connections but $\mathcal{M}^{rc} \neq \mathcal{M}$. Then $\mathcal{M}$ contains a (possibly degenerated) T_4-configuration.* □

For $k = 4$, an attempt was made to solve the system (1) of $4\binom{m}{2}\binom{n}{2} + 8mn$ quadratic and linear equations directly (for some permutation σ of $\{1, 2, 3, 4\}$). But even Gröbner basis methods implemented in *Macaulay 2* failed to solve the system even for simple test cases.

To exploit the algebraic structure, let us define for a matrix $M \in \mathbb{R}^{m\times n}$ its *rank-one cone* $\mathcal{R}_1(M)$ as

$$\begin{aligned} \mathcal{R}_1(M) &:= \{X \in \mathbb{R}^{m\times n} \mid \text{rank}(X - M) \leq 1\} \\ &= \left\{ X \mid \det \begin{pmatrix} X_{rs} - M_{rs} & X_{ru} - M_{ru} \\ X_{ts} - M_{ts} & X_{tu} - M_{tu} \end{pmatrix} = 0, \quad \begin{matrix} 1 \leq r < t \leq m \\ 1 \leq s < u \leq n \end{matrix} \right\}, \end{aligned} \tag{2}$$

i.e., $\mathcal{R}_1(M)$ is the set of all matrices that are rank-one connected to M.

In order to describe $\mathcal{R}_1(M)$ algebraically, the following notation is used. Let $X = (X_{rs})$ be an $m \times n$-matrix of the indeterminates $X_{11}, X_{12}, \ldots, X_{1n}, X_{21}, \ldots, X_{mn}$. The real polynomials in these indeterminates will be denoted by $\mathbb{R}[X]$ (considered as a ring, i.e., addition and multiplication are well defined). Whenever necessary, we will silently identify $\mathbb{R}^{mn}$ and $\mathbb{R}^{m\times n}$. For simplicity, the ideas leading to Algorithm 2.3 will be explained for $\sigma = \mathrm{id}$.

If the matrices $M^{(1)}, \ldots, M^{(k)}$ form a T_k-configuration then the corners of the inner polygon lie necessarily in the intersections of rank-one cones, i.e.,

$$X^{(j)} \in \mathcal{J}_j := \mathcal{R}_1(M^{(j)}) \cap \mathcal{R}_1(M^{(j-1)}),$$

where the index j is counted modulo k. It can be shown that if $m, n \geq 3$ then $\mathcal{J}_j$ is generically empty.

The intersections $\mathcal{J}_j$ $(j = 1, \ldots, k)$ are the zero set of the 2×2-minors of $(X^{(j)} - M^{(j)})$ and $(X^{(j)} - M^{(j-1)})$,

$$\det \begin{pmatrix} X_{rs}^{(j)} - M_{rs}^{(j)} & X_{ru}^{(j)} - M_{ru}^{(j)} \\ X_{ts}^{(j)} - M_{ts}^{(j)} & X_{tu}^{(j)} - M_{tu}^{(j)} \end{pmatrix}, \quad \det \begin{pmatrix} X_{rs}^{(j)} - M_{rs}^{(j-1)} & X_{ru}^{(j)} - M_{ru}^{(j-i)} \\ X_{ts}^{(j)} - M_{ts}^{(j-1)} & X_{tu}^{(j)} - M_{tu}^{(j-1)} \end{pmatrix} \in \mathbb{R}[X^{(j)}],$$

$$1 \leq r < t \leq m, \quad 1 \leq s < u \leq n, \qquad j = 1, \ldots, k \text{ (counted modulo } k). \tag{3}$$

(As a zero set of polynomials, $\mathcal{J}_j$ is by definition a *variety.*) The set of polynomials with the zero set $\mathcal{J}_j$ has the structure of an *ideal* and will be denoted I_j. It is generated by the minors in (3), see, e.g., [5]. If $I_j = \mathbb{R}[X^{(j)}]$, then the associated variety $\mathcal{J}_j$ is empty and there is no candidate point for the corner $X^{(j)}$ of the inner polygon of a possible T_k-configuration.

If $\mathcal{M}$ is a T_k-configuration, then for each j, the matrices $M^{(j)}$, $X^{(j+1)}$ and $X^{(j)}$ lie on a line, in this particular order. This yields the equations and inequalities

$$\lambda_j M^{(j)} + (1 - \lambda_j) X^{(j)} = X^{(j+1)}, \qquad 0 < \lambda_j < 1, \qquad \text{for } 1 \leq j \leq k. \tag{4}$$

In order to describe this in terms of varieties we introduce the polynomial ring $\mathcal{P} := \mathbb{R}[X^{(1)}, \ldots, X^{(k)}, \lambda_1, \ldots, \lambda_k]$ in $kmn + k$ indeterminates. Then we obtain naturally from (4) the polynomials

$$\lambda_j M_{rs}^{(j)} + (1 - \lambda_j) X_{rs}^{(j)} - X_{rs}^{(j+1)} \qquad \text{for } 1 \leq j \leq k,\ 1 \leq r \leq m,\ 1 \leq s \leq n. \tag{5}$$

These kmn polynomials and the polynomials in (3), the latter taken for all $1 \leq j \leq k$, generate an ideal $I \subseteq \mathcal{P}$. For a permutation σ, let I_σ be the ideal generated analogously, with $M^{(j)}$ substituted by $M^{(\sigma^{-1}(j))}$ in (3) and (5). The real variety associated to I_σ will be denoted by $\mathcal{V}_\sigma \subset \mathbb{R}^{kmn+k}$.

With the notation introduced above, $\mathcal{M} = \{M^{(1)}, \ldots, M^{(k)}\} \subset \mathbb{R}^{m\times n}$ is a T_k-configuration if and only if there exists a permutation σ of $\{1, \ldots, k\}$ such that $\mathcal{V}_\sigma \subset \mathbb{R}^{kmn+k}$ contains a point $(X^{(1)}, \ldots, X^{(k)}, \lambda_1, \ldots, \lambda_k)$ with $\lambda_j \in (0, 1)$ for $1 \leq j \leq k$.

The preceding arguments immediately show the correctness of the following algorithm.

Algorithm 2.3

Input: $\mathcal{M} = \{M^{(1)}, \ldots, M^{(k)}\} \subset \mathbb{R}^{m\times n}$ without rank-one connections.

Procedure: For all permutations σ of $\{1, \ldots, k\}$ perform the following test.

1. For $j = 1, \ldots, k$ compute a Gröbner basis for the ideal $I_{\sigma,j}$ generated by the polynomials from (3), with $M^{(j)}$ substituted by $M^{(\sigma^{-1}(j))}$. If $I_{\sigma,j} = \mathbb{R}[X^{(j)}]$ for some j then there exists no solution to (1) for this σ. Else:

2. Compute a Gröbner basis for the ideal generated by the polynomials in (5) with $M^{(j)}$ substituted by $M^{(\sigma^{-1}(j))}$.

3. Compute a Gröbner basis for the ideal I_σ generated by the union of the ideals in Steps 1 and 2. If $I_\sigma = \mathcal{P}$ then there exists no solution to (1) for this σ. Else:

4. Check if there is a a point $(X^{(1)}, \ldots, X^{(k)}, \lambda_1, \ldots, \lambda_k) \in \mathcal{V}_\sigma$ with $\lambda_j \in (0, 1)$ for all $1 \leq j \leq k$. If yes, this is a T_k-configuration; if not, there exists no solution to (1) for this σ.

Output: If $\mathcal{M}$ is a T_k-configuration this is detected in Step 4 for some σ. If $\mathcal{M}$ is not a T_k-configuration, then for every σ, either Step 1, 3 or 4 give a negative answer. □

To perform the check in Step 4, we use a combination of the BKR algorithm [11] and the eliminant method [12]. This requires I_σ to be zero-dimensional in $\mathcal{P}$ (i.e., the complex variety $\mathcal{V}_\sigma \subset \mathbb{C}^{kmn+k}$ has to consist of single points). This was true in every one of the more than 200 000 examples we checked. However, a rigorous proof of the zero-dimensionality is lacking.

Similar ideas can be applied for the detection of degenerated T_k-configurations.

3 Stochastic experiments for T_4-configurations

Extensive tests with random integer matrices in $\mathbb{R}^{2\times 2}, \mathbb{R}^{4\times 2}$ and $\mathbb{R}^{3\times 3}$ have been carried out for $k = 4$. Such computations were not possible with previous methods. Algorithm 2.3 allows for the first time the investigation of stochastic questions, such as the distribution of T_4-configurations in the space of quadruples of matrices. We report some results.

Algorithm 2.3 has been implemented in the computer algebra package *Macaulay 2* [4]. For every experiment, we had *Macaulay 2* generate four random matrices $\mathcal{M} = \{M^{(1)}, M^{(2)}, M^{(3)}, M^{(4)}\}$ with integer entries in the interval $[0, R]$ for $R = 20, 30, 50, 150$. If the set $\mathcal{M}$ was found to have a rank-one connection between two of its elements, the experiment was terminated since such a set $\mathcal{M}$ cannot be a T_4-configuration.

Table 1 shows some results. In particular, almost 9%—a remarkably large number—of all random four-element sets in $\mathbb{R}^{2\times 2}$ were found to form a T_4-configuration. This suggests that the set of all T_4-configurations, considered as a subset of $(\mathbb{R}^{2\times 2})^4$, has positive measure.

Somewhat surprisingly, quite a few *sixfold T_4-configurations* were found. By this term, we mean sets $\mathcal{M}$ that satisfy (1) for *every* permutation σ of $\{1, 2, 3, 4\}$. As shown by Székelyhidi [13, Theorem 3], a T_4-configuration admits a real solution for (1) either for only one σ (up to a rotation) or for all permutations σ. Consistent with this, no twofold or threefold T_4-configurations were found.

As expected, a larger range of entries in the matrices leads to fewer configurations with rank-one connections.

In the cases of $\mathbb{R}^{3\times 3}$ and $\mathbb{R}^{4\times 2}$, no random set of matrices was found to be a T_4-configuration. In $\mathbb{R}^{3\times 3}$, no random configuration yielded four nonempty intersections $\mathcal{J}_j$ of the respective rank-one cones. It was already a rare exception (ca. 0.1% of experiments) to find at least one nonempty intersection. Rank-one cones are five-dimensional objects in a nine-dimensional space; thus this is intuitively not surprising. In $\mathbb{R}^{4\times 2}$, however, the $\mathcal{J}_j$ are two-dimensional, but the ideal I_σ equaled the entire ring $\mathcal{P}$ in every experiment. The complexity of the algorithm increases by necessity for larger k. However, the case $k = 4$ we focussed on is the most interesting and important one for theoretical reasons (see Section 2).

	$\mathbb{R}^{2\times 2}$			$\mathbb{R}^{4\times 2}$	$\mathbb{R}^{3\times 3}$
Range R	30	50	150	50	20
Number of experiments	5 000	50 000	50 000	25 000	100 000
with a rank-one connection	748	776	133	0	0
T_4-configurations	368	4 351	4 392	0	0
thereof sixfold T_4-configurations	2	108	80	0	0
thereof degenerated T_4-configurations	0	0	0	0	0
not a T_4-configuration	3 884	44 873	45 475	25 000	100 000
Average time per experiment on a 1GHz Dual Pentium III	n/a	8.79 s	9.70 s	3.66 s	0.41 s

Table 1: Overview of some results of stochastic experiments

Acknowledgements

This paper contains a part of CFK's Diploma thesis [8], written under the supervision of JZ. The work was carried out while JZ was a postdoctoral scholar at the California Institute of Technology. CFK was a Diploma student in mathematics at the Technische Universität München, Germany and visited Caltech as a special student. His stay was financed by the Freistaat Bayern through a stipend of the Bayerische Begabtenförderung. He thanks Kaushik Bhattacharya for support, and the Division of Engineering and Applied Sciences at Caltech for hospitality. The financial support of an NSF-ITR grant (ACI-0204932) is gratefully acknowledged. We thank Kaushik Bhattacharya for encouragement and generous support.

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